



UNIVERSITÄT ZU LÜBECK

An aerial photograph of Lübeck, Germany, showing the city's red-tiled roofs and the prominent brick towers of the Holtenauer Tor. A large, semi-transparent teal geometric shape, resembling a crystal or a stylized 'K', is overlaid on the bottom half of the image.

34th ANNUAL MEETING
of the GERMAN
CRYSTALLOGRAPHIC
SOCIETY (DGK)

PROGRAMME

25–28 FEBRUARY 2026
LÜBECK

www.dgk-conference.de

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Organisation	4
Welcome note	5
Programme overview	
Wednesday, 25 February	6
Thursday, 26 February	7
Friday, 27 February	8
Saturday, 28 February	9
Scientific programme	
Wednesday, 25 February	11
Thursday, 26 February	16
Friday, 27 February	22
Saturday, 28 February	29
Poster sessions	
Thursday, 26 February	33
Friday, 27 February	39
Social programme	44
Young Crystallographers	46
Meetings of the working groups	48
General information	50
Industrial symposium.....	52
Exhibitors, sponsors and media collaborations	54
Floor plan	55
Index of plenary speakers, authors and chairs	56

ORGANISATION

Venue

University of Lübeck
Audimax
Mönkhofer Weg 245 | 23562 Lübeck (Germany)

Conference website

www.dgk-conference.de

Organiser

German Crystallographic Society (DGK)



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CONGRESSMANAGEMENT



Dear colleagues,

welcome to the 34th Annual Meeting of the German Crystallographic Society (DGK) at University of Lübeck! The conference takes place in the Audimax on the campus of the University of Lübeck located in the south of the city, which can be easily reached by bus in about 20 minutes from the old town or the central station.

The flair of the ancient capital of the Hanseatic League can still be felt today in the old town of Lübeck with its unique skyline of seven Gothic brick church towers, a UNESCO World Heritage Site picturesquely situated on an island in the river Trave. With more than 5,000 students at the university, Lübeck has developed into a young and dynamic student city. Take your time to explore the narrow streets with their bars and restaurants in the typical brick houses. Enjoy the Hosten Gate, of course the world-famous Lübeck marzipan, and, maybe better during summer, the beautiful beaches of the Baltic Sea at Travemünde.

“Focus on life” is the motto of the young and modern University of Lübeck, which offers courses in medicine, natural sciences, computer sciences, and mathematics. Structural biology, particularly the structural analysis of infection-related proteins, has long been the focus of the Institute of Biochemistry, which is hosting this year’s DGK Annual Meeting. To equally represent all areas of crystallography, the program committee was composed of representatives from all DGK working groups. The high scientific quality of the submitted abstracts enabled us to compile a highly interesting and diverse program that will hopefully stimulate discussions, interactions, and knowledge transfer between chemists, physicist, biologists, earth scientists, and material scientists. In addition to six plenary lectures presented by internationally renowned scientists, 18 Microsymposia, and two poster sessions, we invite you to the welcome reception in the foyer of the Audimax and to the conference social evening at the Radisson Blu Senator Hotel directly at the Trave river with a perfect view on the old town. Special highlights will be two symposia honoring the scientific life’s work of George Sheldrick and Rolf Hilgenfeld, two world-renowned crystallographers who sadly passed away in 2025.

Thanks to the DGK executive board for choosing the University of Lübeck as the host for this conference, to the program committee for their excellent work, and to the Conventus team for a perfect cooperation. Special thanks go to the industrial exhibitors, whose support is indispensable for this conference.

Finally, thank you very much for coming to northern Germany from near and far to attend and celebrate the 34th Annual Meeting of the DGK with us! We look forward to your contributions and to an exciting and inspiring conference.

Lars Redecke
Conference Chair

PROGRAMME OVERVIEW | WEDNESDAY, 25 FEBRUARY

AM 1	AM 2	AM 3	AM 4	Building 64, 1 st floor Room 035
				09:00–12:00 DGK Board Meeting p. 11
13:45–14:25 Opening p. 11				
14:30–15:30 Plenary Lecture 1 Claire White p. 11				
15:45–17:05 MS 1 Young Crystallographers: Lightning talks p. 11	15:45–17:15 MS 2 Methods in Structural Biology p. 13	15:45–17:15 MS 3 New Trends and Modelling of Crystal Structures and Properties p. 14	15:45–17:15 MS 4 Crystal Physics p. 15	
17:30–18:30 DGK Honour Evening p. 15				
18:30–19:15 Max Von Laue Award p. 15				
				19:15–21:15 Welcome Reception in the foyer p. 44

PROGRAMME OVERVIEW | THURSDAY, 26 FEBRUARY

AM 1	AM 2	AM 3	AM 4
09:00–10:30 George-Sheldrick-Symposium 1 p. 16	09:00–10:30 MS 5 In Situ/Operando Characterization p. 16	09:00–10:30 MS 6 Crystal Chemistry p. 17	
11:00–12:00 Plenary Lecture 2 Esko Oksanen p. 18			
12:15–13:15 Industrial Symposium p. 52			
13:30–14:30 Plenary Lecture 3 Bo Brummerstedt Iversen p. 18			
14:45–16:15 George-Sheldrick-Symposium 2 p. 18	14:45–16:15 MS 7 Structure-based Drug Discovery p. 19	14:45–16:15 MS 8 Advances and Applications of Neutron and Synchrotron Radiation p. 20	14:45–16:15 MS 9 Synthesis-structure/ Non-crystalline/ Disordered Materials p. 20
16:15–17:45 Poster Session 1 in the foyer p. 33			
17:45–19:45 DGK General Assembly p. 21			
	19:45–21:00 Get Together Young Crystallographers p. 46		

PROGRAMME OVERVIEW | FRIDAY, 27 FEBRUARY

AM 1	AM 2	AM 3	AM 4
08:30–09:30			
Plenary Lecture 4 Pierco Macchi p. 22			
10:00–11:30	10:00–11:30	10:00–11:30	10:00–11:30
MS 10 Non-ambient Conditions and Electron Diffraction Methods p. 22	MS 11 New Biological Structures p. 23	MS 12 New Crystal Structures p. 24	MS 13 Mineralogical Crystallography p. 24
12:15–13:00	12:15–13:00	12:15–13:00	12:15–13:00
Meeting Working Group 6 p. 48	Meeting Working Group 3 p. 48	Meeting Working Group 4 p. 48	Meeting Working Group 2 p. 48
13:00–14:00			
Plenary Lecture 5 Eike C. Schulz p. 25			
14:15–15:45	14:15–15:45	14:15–15:45	14:15–15:15
MS 14 Functional Materials p. 25	MS 15 Time-resolved Crystallography and Protein Design p. 26	MS 16 Frontier Molecular Crystallography and Supramolecular and Framework Structures p. 27	Award Symposium Lieselotte Templeton Award p. 28
15:45–17:15 Poster Session 2 in the foyer p. 39			
17:15–18:00	17:15–18:00	17:15–18:00	17:15–18:00
Meeting Working Group 5 p. 48	Meeting Working Group 9 p. 48	Meeting Working Group 7 p. 48	Meeting Working Group 8 p. 48
19:00–23:00			
Social Evening Radisson Blu Senator Hotel p. 44			

PROGRAMME OVERVIEW | SATURDAY, 28 FEBRUARY

AM 1	AM 2	AM 3
08:45–09:45		
Plenary Lecture 6		
Katharine Page		
p. 29		
09:45–10:00		
Closing		
p. 29		
10:15–12:10	10:15–11:45	10:15–11:45
Rolf-Hilgenfeld-Symposium 1	MS 17	MS 18
	Free Topics	Theory and Software, Data Infrastructure, Big Data and Artificial Intelligence
	p. 29	p. 30
p. 29		
13:00–14:45		
Rolf-Hilgenfeld-Symposium 2		
p. 31		

Opening & Closing
Plenary lecture
Microsymposium
Special lecture
Industrial symposium
Poster session
DGK Internal
Award symposium
Social programme



09:00–12:00 DGK Board Meeting

Building 64,
1st floor,
Room 035

13:45–14:25 Opening

AM 1

14:30–15:30 Plenary Lecture 1

AM 1

Chair R. Neder (Erlangen/DE)

14:30 PL-01

Pair distribution function analysis of cement-based materials: Beyond the standard approach

C. White (Princeton/US)

15:45–17:05 MS 1 | Young Crystallographers: Lightning talks

AM 1

Chair F. Meurer (Regensburg/DE), B. Ebel (Aachen/DE)

15:45 LT-01

PDF analysis of amorphous calcium and magnesium carbonates at high pressures

L. Wedek, L. Bayarjargal (Frankfurt a. M./DE), C. Prescher,

C. Otzen (Freiburg i. Br./DE), K. Glazyrin (Hamburg/DE),

B. Winkler (Frankfurt a. M./DE)

15:50 LT-02

Cs₁₄Hg₁₇O₄ – a new cesium mercuride oxide with a previously unknown [Hg₁₈] cluster

T. Xu, C. Hoch (Munich/DE)

15:55 LT-03

Crystal structures of Cs_{18.5}Rb_{0.5}[AlO₄]₂[Hg₄]₂ and Cs₂₆[Fe₂O₇]₂[Hg]₈[Hg]₆

H. Waldmann, N. Kötter, L. Nusser, C. Hoch (Munich/DE)

16:00 LT-04

Three Polymorphic Modifications of Yb(OAc)₃ Co-existing in the Temperature Range 200-523K: A Relation Between Orthorhombic and Hexagonal Structures

M. Zhernakov, J. Möbs, K. Müller-Buschbaum (Gießen/DE)

- 16:05 **LT-05**
Crystallographic Insights into the Stereoselectivity of Methionine Adenosyltransferases
M. Bolz (Brunswick/DE), L. Gericke, J. Andexer (Freiburg i. Br./DE), W. Blankenfeldt (Brunswick/DE)
- 16:10 **LT-06**
Structural Insights into the ADP Ribosyltransferase (ARR) from *Mycobacterium smegmatis* and the Implications for Inhibitor Search
L. von Soosten (Hamburg/DE)
- 16:15 **LT-07**
 $\text{Ba}_{21}\text{N}_5(\text{MnN}_3)_2$ – a new ternary subnitridometalate
L.-V. Pietsch, C. Hoch (Munich/DE)
- 16:20 **LT-08**
Crystallographic fragment screening towards new NS2B-NS3 Zika protease Inhibitors
L. S. Benz, J. Wollenhaupt, M. Oelker (Berlin/DE), A. Jirgensons (Riga/LV), T. Miletic, U. Müller, M. S. Weiss (Berlin/DE)
- 16:25 **LT-09**
Low-Cost Crystallization Automation for Cationic Metallocavitands (Pillarplexes)
M. Saviak, J. Zuber, L. Richter, A. Pöthig (Garching/DE)
- 16:30 **LT-10**
Cryo and room temperature (RT) serial synchrotron crystallography (SSX) reveals binding modes of previously unexplored β -lactam antibiotics
G. Gore, A. Prester, D. von Stetten, K. Bartels, E. C. Schulz (Hamburg/DE)
- 16:35 **LT-11**
High-throughput structural investigation of Cu content-dependent second phase formation in $(\text{Mn,Fe,Co,Ni,Cu})_3\text{O}_4$ thin film materials libraries
V. Strotkötter, A. Kirsch, A. Ludwig (Bochum/DE)
- 16:40 **LT-12**
Exploring compositional space in non-equipolar high entropy spinel oxides
C. F. Eugenio (Bochum/DE, Bogotá/CO), S. C. Sánchez (Bogotá/CO), A. Kirsch (Bochum/DE)

- 16:45 **LT-13**
Reference Database for Chemical Bonding Analysis
F. Bartley, F. Kleemiß (Aachen/DE)
- 16:50 **LT-14**
Capturing Spin Transitions in Crossover Complexes *via* Quantum
Crystallographic Disorder Refinement
D. Brück, F. Kleemiß (Aachen/DE)
- 16:55 **LT-15**
Porous Pillarplex Materials: Towards Gas Adsorption in the Solid State
J. Zuber, A. Heidecker, A. Pöthig (Garching/DE)
- 17:00 **LT-16**
Crystal architecture through energetic insights: 2,6-bis(4*H*-1,2,4-triazol-4-yl)
pyridine hydrate
M. G. Bogdanović (Novi Sad/RS), I. S. Konovalova (Düsseldorf/DE),
Kharkiv/UA), G. J. Reiss (Düsseldorf/DE), M. V. Rodić (Novi Sad/RS)
- 15:45–17:15 **MS 2 | Methods in Structural Biology**
AM 2
Chair U. Müller (Berlin/DE)
- 15:45 **OP-01**
High-throughput Macromolecular Crystallography at Beamline P11
J. Hakanpää, S. D. Chatziefthymiou, G. Pompidor, A. Grebentsov, A. Gruzinov,
O. Merkulova (Hamburg/DE)
- 16:00 **OP-02**
EMBL Macromolecular Crystallography Facilities at PETRAIII
G. Bourenkov, D. von Stetten, M. Nikolova, M. Agthe, S. Panneerselvam,
D. Ruiz Carrillo, Y. Bloch, K. Kovalev, T. R. Schneider (Hamburg/DE)
- 16:15 **OP-03**
MATTs-PDB: A Dictionary-Based Approach for Aspherical Electron Density
Modeling in Macromolecules
P. Rybicka, M. Kulik (Warsaw/PL), C. Grandgirard (Vandœuvre-lès-Nancy/FR),
M. Chodkiewicz, P. Dominiak (Warsaw/PL)
- 16:30 **OP-04**
Structural Quality and Docking Reliability of Peptide–GPCR Complexes:
A Crystallographic Perspective
S. Jafari, J. Bojarska, W. Wolf (Łódź/PL)

- 16:45 **OP-05**
In situ protein crystallography: a single-crystal electron diffraction pipeline for direct structure determination inside cells, *IncelluloED*
V. Polovinkin (Dolní Břežany/CZ), Š. Bílá (České Budějovice/CZ), D. Pinkas (Prague/CZ), K. Khakurel (Dolní Břežany/CZ), J. Boger (Lübeck/DE), T. Bílý (České Budějovice/CZ), J. Hajdu (Dolní Břežany/CZ, Uppsala/SE), Z. Franta (České Budějovice/CZ), I. de Diego Martinez (Schenefeld/DE), R. Tuma (České Budějovice/CZ), L. Redecke (Lübeck/DE)
- 17:00 **OP-06**
 From nanometer to millimeter: a versatile crystallization approach for electron, X-ray and neutron diffraction
A. Shaikhqasem, F. Hamdi (Halle (Saale)/DE), L. Gajdos, M. P. Blakeley, (Grenoble/FR), P. L. Kastiris, M. T. Stubbs (Halle (Saale)/DE)
- 15:45–17:15 **MS 3 | New Trends and Modelling of Crystal Structures and Properties**
 AM 3
 Chair M. Bodensteiner (Regensburg/DE), R. Herbst-Irmer (Göttingen/DE)
- 15:45 **OP-07**
 How can we trust our crystal structure solutions? *Pseudo*-homometry and chemical reliability in single-crystal X-ray diffraction
A. Virovets (Frankfurt a. M./DE)
- 16:00 **OP-08**
 Accessing new observables via nonlinear crystallography based on x-ray-optical wavemixing
D. Krebs, C. Bömer (Hamburg/DE)
- 16:15 **OP-09**
 T-BAR: Topology-Based Atom Refinement
F. Kleemiß (Aachen/DE), M. Gimferrer (Göttingen/DE)
- 16:30 **OP-10**
 Molecular Dynamics Simulations in Quantum Crystallography: Potentials and Challenges
M. Patzer, C. W. Lehmann (Mülheim an der Ruhr/DE)
- 16:45 **OP-11**
 From Static to Dynamic Polarizabilities: A Transferable Approach to Predict Optical Dispersion in Molecular Crystals
A. Krawczuk, R. Fernandes Ligorio (Göttingen/DE)

- 17:00 **OP-12**
Aspherical modeling: advancing x-ray scattering and sample characterization
K. García Medina, R. Neder (Erlangen/DE)
- 15:45–17:15 **MS 4 | Crystal Physics**
AM 4
Chair E. Haussühl (Frankfurt a. M./DE), M. Münchhalfen (Bochum/DE)
- 15:45 **OP-13**
The impact of ordering phenomena on the physical properties of rare-earth oxoborates $RCa_4O(BO_3)_3$ ($R = Er, Y, Dy, Gd, Sm, Nd, La$), M. Münchhalfen, J. Schreuer (Bochum/DE)
- 16:15 **OP-14**
Phase Evolution, Phase Diagram and Annealing Effects in $V_{1-x}Fe_xO_2$ ($x \leq 1.0\%$) compounds
D. Manousou (Jülich/DE, Athens/GR), S. B. Atata (Athens/GR), Y. J. Sohn, (Jülich/DE), P. Tsipas (Magurele/RO, Athens/GR), A. Grzechnik, (Jülich, Aachen/DE), M. Calamiotou (Athens/GR), K. Frieze (Jülich, Aachen/DE), S. Gardelis (Athens/GR)
- 16:30 **OP-15**
Low-temperature anomalies in elastic properties of single-crystal $(SrAl_{0.5}Ta_{0.5}O_3)_{1-x}(LaAlO_3)_x$
M. Münchhalfen, J. Schreuer (Bochum/DE), C. Gugushev, R. Blukis, A. Ditmar, M. Brützm, S. Ganschow (Berlin/DE)
- 16:45 **OP-16**
Determination of the $Li_2O - K_2O - Ta_2O_5$ phase diagram in the framework of single crystal growth of stoichiometric lithium tantalate
A. Hoffmann, R. Blukis, S. Inckemann, M. Bickermann, S. Ganschow (Berlin/DE)
- 17:00 **OP-17**
Pressure-Driven Depolarization in $BaTiO_3$ Probed by Second Harmonic Generation
T. H. Reuter, L. Bayarjargal (Frankfurt a. M./DE), D. Rytz, S. Schwung, (Idar-Oberstein/DE), V. Milman (Cambridge/GB), B. Winkler (Frankfurt a. M./DE)
- 17:30–18:30 **DGK Honour Evening**
AM 1
- 18:30–19:15 **Max Von Laue Award**
AM 1
- 19:15–21:15 **Welcome Reception in the foyer**
see page 44

09:00–10:30 George-Sheldrick-Symposium 1

AM 1

Chair T. Beck (Hamburg/DE), T. Grüne (Vienna/AT)

09:00 KL-01

George Sheldrick – the man behind SHELX

R. Herbst-Irmer (Göttingen/DE)

09:30 KL-02

In Honour of George Sheldrick. Small Molecule Software: SHELX and the passing of the torch

L. Bourhis (Marne-la-Vallée/FR)

10:00 KL-03

In Honour of George Sheldrick. Methods Development in Crystallography

A. Thorn (Berlin/DE)

09:00–10:30 MS 5 | In Situ/Operando Characterization

AM 2

Chair H. Prell (Berlin/DE)

09:00 OP-18

Exploring the World of Carbonates: Mechanochemical Synthesis and In Situ X-ray Powder Diffraction (XRPD) Studies

H. Das, C. Weidenthaler (Mülheim an der Ruhr/DE), V. Kahlenberg (Innsbruck/AT)

09:15 OP-19

In situ H₂/D₂ sorption study of Zinc-based CALF-20 by XRPDA. Sleptsova, S. Bette, P. Sarkar, M. Hirscher, F. Adams,

R. E. Dinnebier (Stuttgart/DE)

09:30 OP-20

In Situ Investigation of Fluorination Pathways in Ruddlesden-Popper OxyfluoridesJ. Jacobs, J. Geßner, S. G. Ebbinghaus (Halle (Saale)/DE)

09:45 OP-21

Temperature-dependent phase transition in high-efficiency hybrid halide perovskites

A. Palacios Saura, D. M. Többsen, S. Schorr (Berlin/DE)

- 10:00 **OP-22**
In situ XRPD investigations on the reduction of iron oxide and sodium chromate by hydrogen
M. Häger, H. Kohlmann (Leipzig/DE)
- 10:15 **OP-23**
 Multimetallic nanoparticle exsolution from high-entropy spinels
 G. B. Strapasson (Campinas/BR, Copenhagen/DK),
 K. M. Ø. Jensen (Copenhagen/DK), D. Zanchet (Campinas/BR),
A. Kirsch (Bochum/DE)
- 09:00–10:30 **MS 6 | Crystal Chemistry**
 AM 3
 Chair J. Breternitz (Steinfurt/DE), T. Leisegang (Freiberg/DE)
- 09:00 **OP-24**
 Structures and properties of new multinary bismuth subiodides with intermetallic nanoribbons and chains
 N. G. Elsner (Dresden/DE)
- 09:15 **OP-25**
 Extending the coordination number rule – A comparison of the results for ternary fluorides, chlorides, bromides, iodides and oxides
N. Langer, H. Kohlmann (Leipzig/DE)
- 09:30 **OP-26**
 Flexible carbodiimide and dicyanometallate frameworks – Coupling negative thermal expansion and negative linear compressibility in wine-rack-like structures
A. Corkett (Jülich/DE), K. Frieze, A. Grzechnik (Jülich, Aachen/DE)
- 09:45 **OP-27**
 Superstructures of Se-substituted bornite-type $\text{Cu}_5\text{-xFeS}_4\text{-ySe}_y$
P. Sicher, O. Oeckler, C. Fraunhofer (Leipzig/DE)
- 10:00 **OP-28**
 High-pressure synthesis and structural studies of nitride perovskites ABN_3 (A = Pr, Nd, B = W, Re)
F. I. Akbar (Frankfurt a. M./DE), S. D. Kloß (Munich/DE),
 M. Bykov (Frankfurt a. M./DE)

10:15	OP-29 Crystal structures of alkali oxidohydroxidoantimonates (Na, K, Rb, Cs) and of NaSbO ₂ comprising anionic chains and sheets <u>T. Wölflechner</u> , M. Weil (Vienna/AT)
11:00–12:00	Plenary Lecture 2
AM 1	
Chair	J. Hakanpää (Hamburg/DE)
11:00	PL-02 Macromolecular Crystallography at the European Spallation Source E. Oksanen (Lund/SE)
12:15–13:15	Industrial Symposium Bruker AXS GmbH
AM 1	see page 52
13:30–14:30	Plenary Lecture 3
AM 1	
Chair	F. Kleemiß (Aachen/DE)
13:30	PL-03 Disorder in thermoelectric materials B. Brummerstedt Iversen (Aarhus C/DK)
14:45–16:15	George-Sheldrick-Symposium 2
AM 1	
Chair	A. Thorn (Berlin/DE), R. Herbst-Irmer (Göttingen/DE)
14:45	KL-04 From crystallography to school – and back E. Irmer (Göttingen/DE)
15:05	KL-05 Core Facility run by a SHELXL power user T. Grüne (Vienna/AT)
15:25	KL-06 The magic triangle and beyond: Insights from doing a PhD with George Sheldrick T. Beck (Hamburg/DE)

- 15:45 **KL-07**
Refining Large and Complex Molecular Structures with SHELXL
J. J. Holstein (Dortmund/DE)
- 16:05 Discussion
- 14:45–16:15 **MS 7 | Structure-based Drug Discovery**
AM 2
Chair S. Knapp (Frankfurt a. M./DE)
- 14:45 **OP-30**
X-ray fragment screening towards the development of novel cathepsin inhibitors
S. Falke, S. Günther, J. Lieske, P. Reinke, T. Schulze, C. Ehrt, N. Schulz, M. Rarey (Hamburg/DE), K. Karničar, D. Turk (Ljubljana/SI), A. Meents (Hamburg/DE)
- 15:00 **OP-31**
Targeting the methylerythritol phosphate pathway (MEP), via the 1-deoxy-D-xylulose 5-phosphate reductoisomerase (DXR), using a fragment-based drug design approach
S. D. Chatziefthymiou (Hamburg/DE), F. Gerteis, T. Szal (Hamburg, Bremen/DE), J. Hakanpää (Hamburg/DE), B. Windshügel (Hamburg, Bremen/DE)
- 15:15 **OP-32**
Room-temperature X-ray fragment screening with serial crystallography
S. Günther, P. Fischer, M. Galchenkova, S. Falke, P. Reinke, S. Thekku Veedu, A. C. Rodrigues, J. Senst, D. Elinjikkal, L. Gumprecht, J. Meyer, H. Chapman, M. Barthelmess, A. Meents (Hamburg/DE)
- 15:30 **OP-33**
Accelerating Drug Discovery with Home-Lab SC-XRD
V. Smith, A. Lübben, T. Dunaj, M. Adam (Karlsruhe/DE)
- 15:45 **OP-34**
Crystallographic analysis of EnT-derived 3D boron heterocycles reveals covalent Ser70 binding in CTX-M-14 β -lactamase, mimicking the hydrolysis transition state and highlighting their potential as next-generation boronate inhibitors
M. Perbandt (Hamburg/DE), H. M. Kortman, H. Fang, K. A. C. Bastick, C. Völkel (Potsdam/DE), D. Oberthür, T. Beck (Hamburg/DE), P. H. Seeberger, J. J. Molloy (Potsdam/DE)

- 16:00 **OP-35**
Structural and functional analysis of MqnB from *Helicobacter pylori*
S. Korn, A. Prasad, D. A. Nguyen, C. Breithaupt, M. T. Stubbs (Halle (Saale)/DE)
- 14:45–16:15 **MS 8 | Advances and Applications of Neutron and Synchrotron Radiation**
AM 3
Chair M. Etter (Hamburg/DE), M. Meven (München/DE)
- 14:45 **OP-36**
Structures of Ices by Quantum Crystallography and PDF
K. Wozniak, W. Sławiński, G. Łach, R. Gajda, M. Chodkiewicz, P. Reinhard, M. Arhangelskis (Warsaw/PL), C. Ridley (Oak Ridge, TN/US, Chilton/GB), C. Bull (Edinburgh, Chilton/GB)
- 15:30 **OP-38**
Special effects – Verification of corrections for absorption, anomalous dispersion and polarisation
M. Bodensteiner (Regensburg/DE), C. Hennig (Dresden/DE, Grenoble/FR), F. Meurer (Regensburg/DE)
- 15:45 **OP-39**
FIREPOD: A new thermal high-throughput powder diffractometer at MLZ
C. Hauf, M. Hölzel, A. Senyshyn, P. Wagner (Garching/DE)
- 16:00 **OP-40**
ASAXS in Material Science and presentation of some analysis techniques with a software tool
A. Hoell, N. Huseyn-zada, S. Schorr (Berlin/DE)
- 14:45–16:15 **MS 9 | Synthesis-structure/Non-crystalline/Disordered Materials**
AM 4
Chair S. Bette (Stuttgart/DE)
- 14:45 **OP-41**
Revealing the Structure of Water by Variable Temperature Diffraction
J. D. Martin (North Carolina/US)
- 15:00 **OP-42**
A Peptide-Based Porous Coordination Polymer with Ultrahigh Water-Alcohol Selectivity
K. Papadopoulos (Dresden/DE), B. Mazur (Wrocław/PL), S. Ehrling, (Leipzig/DE), A. Mosberger (Dresden/DE), B. Kuchta (Wrocław/PL), V. Bon, S. Kaskel (Dresden/DE)

- 15:15 [OP-43](#)
Pressure-induced nonmetal–metal transition between SnI_4 amorphous states
K. Fuchizaki (Matsuyama/JP)
- 15:30 [OP-44](#)
Synthesis, properties and local structure analysis of the mineral strätlingite
[A. Shevchenko](#) (Stuttgart/DE), M. W. Terban (Mannheim/DE), R. E. Dinnebier,
S. Bette (Stuttgart/DE)
- 15:45 [OP-45](#)
Synthesis and performance analysis of novel nanocomposite-based
Hydroxyapatite in agriculture
[I. Adouar](#), S. Herradi, S. Rakib, B. El Bali, M. Lachkar (Fez/MA)
- 16:00 [OP-46](#)
New structural insights and unexpected developments in boron compounds
[A. Piekara](#), W. Sławiński (Warsaw/PL)
- [16:15–17:45](#) [Poster Session 1](#)
Foyer see page 33
- [17:45–19:45](#) [DGK General Assembly](#)
AM 1
- [19:45–21:00](#) [Get Together Young Crystallographers](#)
AM 2 see page 46

08:30–09:30 Plenary Lecture 4

AM 1

Chair A. Krawczuk (Göttingen/DE)

08:30 PL-04

The subtle exchange mechanism in magnetic coordination polymers at ambient and non-ambient conditions

P. Macchi (Milano/IT)

10:00–11:30 MS 10 | Non-ambient Conditions and Electron Diffraction Methods

AM 1

Chair M. Etter (Hamburg/DE), M. Meven (München/DE)

10:00 OP-47

Extreme Conditions, Extraordinary Insights, Safe Operation: New SC-XRD High-Temperature Device (HTD) for temperatures up to 1300 K

T. Stürzer, A. Lübben, M. Adam (Karlsruhe/DE)

10:30 OP-48

Platform for Swift Heavy Ion Irradiation under Extreme Pressure Conditions: Design for Extending to Cryogenic and High-Temperature Regimes

T. H. Reuter, L. Bayarjargal (Frankfurt a. M./DE), I. Tzifas (Darmstadt/DE), J. Liang (Frankfurt a. M./DE), P. Simon, K.-O. Voss (Darmstadt/DE), C. Schröck (Frankfurt a. M., Darmstadt/DE), C. Trautmann, M. E. Toimil-Molares (Darmstadt/DE), B. Winkler (Frankfurt a. M./DE)

10:45 OP-49

iSFAC modelling: Experimental determination of partial charges with electron diffraction

T. Grüne, S. Mahmoudi, C. Schröder (Vienna/AT)

11:00 OP-50

Variable temperature diffraction and polymorph screening with the XtaLAB Synergy-ED

E. Buchsteiner, K.-N. Truong (Neu-Isenburg/DE), R. Bücker, (Neu-Isenburg/DE, Tokyo/JP), C. Göb (Singapore/SG), C. J. Schürmann, J. Wojciechowski (Neu-Isenburg/DE), M. Jasnowski, M. Meyer (Wrocław/PL), F. White (Neu-Isenburg/DE, Tokyo/JP)

11:15 OP-51

Electron diffraction for everyone: classic and new 3DED protocols in Instamatic

D. Tchoń, L. Palatinus (Prague/CZ)

10:00–11:30 MS 11 | New Biological Structures

AM 2

Chair G. Weber (Berlin/DE)

10:00 OP-64

Racemic crystal structure of a synthetic DNA hairpin with diquinoline linker
P. Mandal (Klosterneuburg/AT), M. Loos, F. Xu, I. Huc (Munich/DE)

10:15 OP-65

How Nature Powers Alkane Monooxygenases: Understanding the Electron Transfer in AlkB Complexes with Different Architectures
I. Span, R. Ganguly, K. Parashar (Erlangen/DE), R. Austin (New York City, NY/US)

10:30 OP-66

Molecular basis for azetidine-2-carboxylic acid biosynthesis
T. Klaubert, J. Gellner (Garching/DE), J. Effert (Marburg/DE), V. Kaila, (Stockholm/SE), H. Bode (Marburg/DE), Y. Li (Paris/FR), M. Groll (Garching/DE)

10:45 OP-67

Discovery of Arg-Cys and Gly-Cys N-O-S Linkages in Proteins via Machine-Learning and QM-Refined Structural Re-analysis
S. Bazzi (Hamburg/DE), S. Sayyad (Pullman, WA/US)

11:00 OP-68

Cryo-EM Structure of an Acyl-CoA Carboxylase Complex Essential for Mycolic Acid Synthesis in Mycobacteria
S. Geibel (Leiden/NL)

11:15 OP-69

Structural Insights into Transcription Regulation by ECF sigma factors in CRISPR Antiviral Defense
S. Binder, N. Schneberger (Bonn/DE), T. Heidler, S. Shahzad, D. Mann (Jülich/DE), M. Geyer, G. Hagelueken (Bonn/DE)

10:00–11:30 MS 12 | New Crystal Structures

AM 3

Chair T. Doert (Dresden/DE)

10:00 OP-58

Copper bismuth iodide – a photovoltaic compound with convoluted structural classification

D. M. Töbrens (Berlin/DE), R. Datta, A. Colsmann, H. Röhm (Karlsruhe/DE), S. Schorr (Berlin/DE)

10:15 OP-59

Pressure-induced formation of compounds in the Re-S binary system

N. Sharapova, V. Kovalev, D. Spahr, B. Winkler (Frankfurt a. M./DE), N. Giordano (Hamburg/DE), E. Bykova (Frankfurt a. M./DE)

10:30 OP-60

Oxidomercurates of alkali metals – crystal structures and chemical bonding
C. Hoch (Munich/DE)

10:45 OP-61

Structure Determination from Phase Mixtures by High-Throughput Electron Diffraction

C. Jandl, J. Merkelbach, D. Stam, G. Steinfeld, G. Santiso-Quinones (Allschwil/CH)

11:00 OP-62

Coordination Chemistry of Catechol-Functionalized TREN Ligand Systems

B. Ebel, G. Hempelmann, I. M. Oppel (Aachen/DE)

11:15 OP-63

(Poly-)Chalcogenides: From binary salts to complex Solvates
G. Thiele (Freiburg i. Br./DE)

10:00–11:30 MS 13 | Mineralogical Crystallography

AM 4

Chair E. M. Schmidt, M. Fischer (Bremen/DE)

10:00 OP-52

Mineral–organic crystalline superstructures in biogenic glass assemblies

I. Zlotnikov (Dresden/DE)

10:15 OP-53

The structure of calcium phosphate nanoparticles in comparison to biogenic and geological calcium phosphate

M. Epple, K. Kostka-Wirtz, K. Loza, O. Prymak (Essen/DE)

10:30	OP-54 Deminerlization and remineralization of tooth enamel from a chemical perspective <u>M. Epple</u> (Essen/DE), J. Enax, E. Schulze zur Wiesche (Bielefeld/DE)
10:45	OP-55 The role of volatiles in the stabilization of iron-rich compounds at high pressures <u>V. Kovalev</u>, N. Sharapova (Frankfurt a. M./DE), X. Li (Grenoble/FR), C. Longa (Milan/IT), D. Spahr (Frankfurt a. M./DE), A. Pakhomova (Grenoble/FR), B. Winkler (Frankfurt a. M./DE), V. Cerantola (Milan/IT), E. Bykova (Frankfurt a. M./DE)
11:00	OP-56 Itelmenite-related $A^{+2}M^{2+3}(SO_4)_4$ sulfates: new representatives and structural classification A. Borisov (Kiel/DE), I. Pimshin (Saint Petersburg/RU), A. Holzheid (Kiel/DE), D. Charkin (Moscow/RU)
11:15	OP-57 Structural changes in $CaSiO_3$ glass up to lower mantle pressures <u>C. Prescher</u>, C. Otzen, G. Cocomazzi (Freiburg i. Br./DE), K. Glazyrin, H.-P. Liermann (Hamburg/DE)
12:15–13:00	Meeting Working Groups see page 48
13:00–14:00	Plenary Lecture 5
AM 1	
Chair	L. Redecke (Lübeck/DE)
13:00	PL-05 Time-resolved serial crystallography: watching enzymes at work E. C. Schulz (Hamburg/DE)
14:15–15:45	MS 14 Functional Materials
AM 1	
Chair	A. Kirsch (Bochum/DE)
14:15	OP-70 Impact of Intrinsic point defects on the performance of CZTS Monograin solar cells <u>H. Prell</u>, G. Gurieva, S. Schorr (Berlin/DE)

- 14:30 **OP-71**
Structural relations in chalcogenide compound semiconductors for photovoltaic applications
S. Schorr, G. Gurieva (Berlin/DE)
- 14:45 **OP-72**
Crystallographic Investigation of Intermediates in the Synthesis of Alkaline Earth Metals Tetrahydroborates
A. Sedykh (Leipzig/DE)
- 15:00 **OP-73**
Structural and compositional design of layered oxide cathodes for sodium batteries
D. Mikhailova (Eggenstein-Leopoldshafen/DE)
- 15:15 **OP-74**
Fractal metal structures for battery electrodes: Morphology, microstructure, application
T. Leisegang, S. von Bahder, M. Momeni, Y.-M. Li, H. Morhli, M. Danziger (Freiberg/DE)
- 15:30 **OP-75**
3D electron diffraction mapping of perturbations in van der Waals gap tailored non centrosymmetric elastic molecular crystals
S. Dey, M. Jarošová, H. Chintakindi, V. Eigner, L. Palatinus (Prague/CZ)
- 14:15–15:45 **MS 15 | Time-resolved Crystallography and Protein Design**
AM 2
Chair E. C. Schulz (Hamburg/DE)
- 14:15 **OP-76**
Catalytic dynamics in an antibiotic resistance enzyme observed by time-resolved crystallography
R. Bosman, E. C. Schulz (Hamburg/DE)
- 14:30 **OP-77**
Structural characterization of the BLUF photoreceptor OaPAC using time-resolved crystallography and FTIR spectroscopy
A. Chretien (Schenefeld/DE), M. Nagel (Bielefeld/DE), S. Botha (Tempe, AZ/US), D. von Stetten (Hamburg/DE), R. de Wijn (Schenefeld/DE), P. Mehrabi (Hamburg/DE), A. Mancuso, J. Schulz (Schenefeld/DE), A. Pearson (Hamburg/DE), T. Kottke (Bielefeld/DE), K. Lorenzen, R. Schubert (Schenefeld/DE)

- 14:45 **OP-78**
Implementing electric field-stimulated X-ray crystallography at EMBL P14 T-REXX using Hadamard time-resolved X-ray crystallography
M. Klureza, J. Estengre Pérez, E.-E. Römer (Hamburg/DE), Y. Pulnova, (Dolní Břežany/CZ), C. D. Gaman (Leeds/GB), F. Tellkamp, J.-P. Leimkohl, M. Kollwe, M. Nikolova, H. Schikora (Hamburg/DE), G. Beddard (Leeds/GB), G. Bourenkov, D. von Stetten (Hamburg/DE), D. Hekstra (Cambridge, MA/US), B. Yorke (Leeds/GB), A. Pearson (Hamburg/DE)
- 15:00 **OP-79**
Enzymes for a sustainable plastic waste management
P. Singh, Y. Boyakova, C. Genter-Dieiguez, P. Da Silva, T. Bock-Bierbaum, M. S. Weiss, F. Lennartz, G. Weber (Berlin/DE)
- 15:15 **OP-80**
From Protein Design to Crystalline Biohybrids: Building Ordered Superlattices
T. Beck (Hamburg/DE)
- 15:30 **OP-81**
Structure based development of new E3 Ligase Ligands
S. Knapp (Frankfurt a. M./DE)
- 14:15–15:45 **MS 16 | Frontier Molecular Crystallography and Supramolecular and AM 3 Framework Structures**
Chair A. Pöthig (Garching/DE), N. Nöthling (Mülheim a. d. Ruhr/DE)
- 14:15 **OP-82**
How many isomers hide within the disordered core of a supramolecule?
E. Peresypkina (Frankfurt a. M./DE)
- 14:30 **OP-83**
Photocrystallography Setup and In Crystallo Photoreaction:
A Novel Approach to Study Light-Induced Chemical Processes
J. J. Holstein (Dortmund/DE)
- 14:45 **OP-84**
Effect of Solvent on the Spin Crossover and Aging Process in $[\text{Fe}(\text{NQu})_3(\text{NCS})_2]$
P. Prakash, H. Shahed (Jülich/DE), H. Hüppe (Aachen/DE), W. Zhou (Jülich, Aachen/DE), J. Qi (Jülich/DE), A. Grzechnik (Aachen, Jülich/DE), J. Voigt, M. Angst, J. Perßon (Jülich/DE), B. Gasharova, Y.-L. Mathis (Karlsruhe/DE), D. Chernyshov (Grenoble/FR), K. Frieße (Jülich, Aachen/DE)

- 15:00 **OP-85**
Synthesis and characterization of a novel Ni-coordination polymer within the framework of a high school research project
S. Bette, T. Pal (Stuttgart/DE), J. Guo (Heidelberg/DE), B. V. Lotsch (Stuttgart/DE)
- 15:15 **OP-86**
Exploring Endohedral and Exohedral Weak Interactions of Pillarplex-Based Nanotubes
A. Pöthig (Garching/DE)
- 15:30 **OP-87**
Occupancy determination from Anomalous Dispersion Refinement
F. Luiz Alves Jardim (Regensburg/DE, Belo Horizonte/BR), J. Figueiredo, C. Pinheiro (Belo Horizonte/BR), M. Bodensteiner (Regensburg/DE)
- 14:15–15:15 AM 4 **Award Symposium – Lieselotte Templeton Award Symposium of the Young Crystallographers**
- 15:45–17:15 **Poster Session 2**
Foyer see page 39
- 17:15–18:00 **Meeting Working Groups**
see page 48
- 19:00–23:00 **Social Evening at ‚Radisson Blu Senator Hotel‘**
see page 44

08:45–09:45 Plenary Lecture 6

AM 1

Chair A. Kirsch (Bochum/DE)

08:45 PL-06

Compositionally Complex Oxides: A Modern Frontier

K. Page (Oak Ridge, Tennessee/US)

09:45–10:00 Closing

AM 1

10:15–12:10 Rolf-Hilgenfeld-Symposium 1

AM 1 You can find the related programme information in the online programme.

10:15–11:45 MS 17 – Free topics

AM 2

Chair R. Neder (Erlangen/DE)

10:15 OP-88

New Software Tools for Teaching Crystallography to a Broader Audience

T. Dunaj, C. Lenczyk, T. Stürzer, A. Lübben, J. Luebben (Karlsruhe/DE)

10:30 OP-89

Making chemical bonds experimentally visible – From residual electron density to bond characteristics

E. Irmer, R. Herbst-Irmer (Göttingen/DE)

- 10:45 **OP-90**
From Research to Education: Teaching Crystallography with the Bilbao Crystallographic Server
G. de la Flor (Karlsruhe/DE), E. Tasci (Ankara/TR), L. Elcoro, J. M. Perez-Mato, G. Madariaga, M. I. Aroyo (Bilbao/ES)
- 11:00 **OP-91**
Crystallography is more than X-ray diffraction – 2 years of teaching fundamental crystallography to chemical engineering students
J. Breternitz (Steinfurt/DE)
- 11:15 **OP-93**
The thermodynamic limit as criterion to derive a crystal structure model
A. Leineweber (Freiberg/DE)
- 11:30 **OP-94**
Energy as the architect: Decoding the supramolecular design of pyrazinamide polymorphs
I. S. Konovalova (Düsseldorf/DE, Kharkiv/UA), G. J. Reiss (Düsseldorf/DE)
- 10:15–11:45 **MS 18 | Theory and Software, Data Infrastructure, Big Data and Artificial Intelligence**
AM 3
Chair F. Kleemiß (Aachen/DE), A. Krawczuk (Göttingen/DE)
- 10:15 **OP-95**
Analytic Scattering Factor Calculation by Direct Partitioning using Density Fitting
L. M. Seifert, F. Kleemiß (Aachen/DE)
- 10:30 **OP-96**
Closed-form expressions of one-dimensional diffuse scattering and what we can learn from them
B. Stöger (Vienna/AT)
- 10:45 **OP-97**
D3A: Direct DOI Dataset Access – Streamlining Data Discovery in the OSCARS Project
M. Nentwich (Hamburg/DE), I. Akhundov (Bremen/DE), P. Fuhrmann, A. P. Millar (Hamburg/DE)

- 11:00 **OP-98**
CRYSTRAC: CIF File Batch Processing for Structural Analysis
D. Ngo (Washington, D.C./US), S. M. Morrison (Piscataway, NJ/US),
A. Prabhu (Washington, D.C./US), J.-M. Hübner (Dresden/DE)
- 11:15 **OP-99**
Quantum crystallography and anomalous dispersion refinement of actinide
Compounds
F. Meurer (Regensburg/DE), S. T. Liddle (Manchester/GB),
M. Bodensteiner (Regensburg/DE)
- 11:30 **OP-100**
Linearization Routines for the Parameter Space Concept to determine
Crystal Structures without Fourier Inversion
M. Vallinayagam (Dresden, Freiberg/DE), M. Nentwich (Hamburg/DE),
D. C. Meyer (Freiberg/DE), M. Zschornak (Dresden, Freiberg/DE)
- 13:00-14:45 **Rolf-Hilgenfeld-Symposium 2**
AM 1 You can find the related programme information in the online programme.



Advances and Applications of Neutron and Synchrotron Radiation

- PP-01 Pressure-induced breakdown of the defect superstructure of $\text{GdTe}_{1.8}$
T. Doert (Dresden/DE), R. Loriga Jr., E. Carvajal (Miami, FL/US),
 G. S. Nolas (Tampa, FL/US), S. Chariton, V. Prakapenka (Chicago, IL/US),
 I. Chuvashova (Miami, FL/US)

New Trends and Modelling of Crystal Structures and Properties

- PP-02 Bridging Quantum Crystallography and Experimental Charge Density Analysis
 through an Iterative Multipole Refinement Scheme
M. Patzer, C. W. Lehmann (Mülheim an der Ruhr/DE)

Theory and Software, Data Infrastructure, Big Data and Artificial Intelligence

- PP-04 X-Area, Integrate3D and ViewSpace: Better Views, Outstanding Data Quality,
 Same Reliable Software
L. C. Folkers-Karlsson, P. Celani (Darmstadt/DE)
- PP-05 On the artificial crystal structure generation for solving the phase problem
 with deep learning
D. M. Melgalvis (Riga/LV), T. Rekis (Riga/LV, Frankfurt a. M./DE)
- PP-06 Streamlined Structure Determination using PROTEUM and CCP4
A. Lübben, J. Luebben, T. Dunaj (Karlsruhe/DE)
- PP-07 Data analysis and gap reconstruction: an application to powder
 diffraction data
K. García Medina, R. Neder (Erlangen/DE), E. Estévez Rams (La Habana/CU)

Methods in Structural Biology

- PP-08 Facilities for Macromolecular Crystallography at the HZB
U. Müller, M. S. Weiss (Berlin/DE)
- PP-09 Mass Spectrometry Platform as Sample Delivery System for Gas-phase
 Small-angle X-ray scattering (SAXS) Experiments
J. C. K. Kung (Hamburg, Lübeck/DE), T. Kierspel (Hamburg/DE),
 T. Damjanovic, S. Mishra, C. Uetrecht (Hamburg, Lübeck/DE)
- PP-11 Structural and Dynamic Characterisation of Phloem-Mobile Protein-RNA
 condensates
S. Smitha, D. P. Triandafillidis, S. Ostendorp, A. Pearson, J. Kehr,
 A. Madsen (Hamburg/DE)

- PP-88 Time-resolved electron diffraction: a method for imaging membrane proteins in action
J. Estengre Pérez, P. Christian, A. Pearson, I. Fernandez-Cuesta, N. Pranzner, J. Teuber (Hamburg/DE)
- Structure-based Drug Discovery
- PP-12 An X-ray based fragment screening approach to develop new antibacterial drugs
A.-M. Herzog, M. Zeno (Stuttgart/DE), D. Stegmann (Stuttgart/DE), Villigen/CH), T. Barthel, M. S. Weiss, J. Steuber, G. Fritz (Stuttgart/DE)
- PP-13 Structural and functional features of a conserved DNA-binding domain in herpesviral proteins as a basis for innovative targeted therapies
F. A. Sornaly (Lübeck/DE), M. M. Brinkmann (Brunswick/DE), T. F. Schulz (Hanover/DE), L. Redecke (Lübeck/DE)
- PP-14 Targeting Flavin Transferase with Fragment-Based Drug Discovery to Address Antimicrobial Resistance
M. Zeno, J. Vering (Stuttgart/DE), T. Barthel, M. S. Weiss (Berlin/DE), J. Steuber, G. Fritz (Stuttgart/DE)
- PP-15 Structural investigation of UL3 from herpes simplex virus type 1: A structural homolog of a conserved DNA-binding protein domain in herpesviral proteins?
A. Weißenburg (Lübeck/DE), T. F. Schulz (Hanover/DE), M. M. Brinkmann (Brunswick/DE), L. Redecke (Lübeck, Hamburg/DE)
- PP-16 Crystallographic analysis of the human FTase β -subunit isoforms will complete kinetic and structural characterization
D. C. Rittmann, M. C. Kehrenberg, A. Hagemann, H. Bachmann (Witten/DE)
- PP-17 MTAN as an anti-virulence drug target – first insights via crystallographic fragment screening
L. Schenkman, M. Oelker, T. Barthel, F. Lennartz, L. S. Benz, M. S. Weiss (Berlin/DE)
- PP-92 Structural and Biophysical Characterization of Complement Control Protein of Kaposi's Sarcoma Associated Herpes Virus
H. Fatima, G. Ssebyatika (Lübeck/DE), N. Plückebaum, C. Jürgens (Hannover/DE), B. Husain (South San Francisco/US), L. Mendes Monteiro (Hannover/DE), N. Martinez-Martin (South San Francisco/US), A. Viejo-Borbolla (Hannover/DE), T. Krey (Lübeck/DE)

New Biological Structures

- PP-18 Structural and spectroscopic characterisation of AlkB domains involved in electron transfer during alkane oxidation
R. Ganguly, K. Parashar, I. Span (Erlangen/DE)
- PP-19 Interplay of Proton-Coupled Electron Transfer and Enzyme Dynamics in Pyruvate Oxidase
F. Rabe von Pappenheim, S. Bartel, K. Tittmann (Göttingen/DE)
- PP-20 Structural and biochemical characterization of regulation and function of the Rab23 GTPase
N. Elagouri, S. Wilmes, D. Kümmel (Münster/DE)
- PP-21 Structural insights into transcription regulation by Mating factor proteins
P. Soumitra (Bochum/DE)

Crystal Chemistry

- PP-22 Two new Ba/Li gallides with $[Ga_2]$ dumbbells: $Ba_2Li_2[Ga_2]$ and $BaLi_8[Ga_4][Ga_2]$
M. Otteny, Q. Da Cruz, M. Wendorff, C. Röhr (Freiburg i. Br./DE)
- PP-23 Novel Oxygen-Rich Phases in Alkali and Alkaline Earth Metal Oxides under Extreme Conditions
J. Lyu, B. Winkler, D. Spahr, E. Bykova, L. Brüning, R. Akilli, F. I. Akbar, M. Bykov (Frankfurt a. M./DE)
- PP-24 $Tl_2Cu_2As_2S_5$, a new mineral with a unique 2D structure
S. Graeser (Kopenhagen/DK), D. Topa (Vienna/AT, Kopenhagen/DK), H. Effenberger (Vienna/AT), E. Makovicky (Copenhagen/DK), W. H. Paar G. Dincă (Bucharest/RO)

New Crystal Structures

- PP-25 Design and synthesis of new photoluminescent coordination polymers employing a ligand derived from quinoline and pyridine
A. Kochel (Wrocław/PL), M. Hołyńska (Noordwijk/NL)
- PP-26 Synthesis and crystal structure of a new hydrous scandium carbonate $Sc[HCO_3][CO_3]$
J. Bungarten, L. Bayarjargal, D. Spahr, N. Sharapova, Y. Wang (Frankfurt a. M./DE), V. Milman (Cambridge/GB), B. Winkler (Frankfurt a. M./DE)

- PP-27 Discovery of inorganic tricarbonat salt: high-pressure synthesis and structure of $K_2C_3O_7$
A. Aslandukov (Frankfurt a. M./DE)
- PP-28 Coinage metal complexes of a dehydrobenzo[16]annulene derivative: superstructures, diffuse scattering and intermolecular interactions
M. Koohgard, M. Tamm, D. Bockfeld, C. Kleeberg (Brunswick/DE)
- PP-29 $K_3Tm_7S_{12}$: Another Potassium Lanthanoid(III) Sulfide with $Cs_3Y_7Se_{12}$ -Type Crystal Structure
K. Engel, T. Schleid (Stuttgart/DE)
- PP-30 $\{Yb[N(CN)_2]_2(H_2O)_4\}Cl \cdot H_2O$: The First Mixed-Anionic Dicyanamide Hydrate
R. J. C. Locke, O. Reckeweg, T. Schleid (Stuttgart/DE)
- PP-31 Structure Elucidation of Liquids Using Organic Crystallization Chaperones
J. Hartenfels, T. Berking, G. L. Runge-Seither, W. Frey, C. Richert (Stuttgart/DE)
- PP-32 Expanding the Coordination Mode Space of Calix[4]imidazolium[2]pyrazole
B. Bock (Neufahrn b. Freising, Munich/DE), S. Deger, T. Pickl, J. Preinl, S. Inoue, A. Pöthig (Munich/DE)
- PP-33 Beyond simple octahedral layers of Ruddlesden-Popper (RP) and Dion-Jacobson (DJ) phases: New mixed Ag^+/Bi^{3+} bromido metalates with organic ammonium cations
C. Schweinle, M. Ade, M. Daub, C. Röhr (Freiburg i. Br./DE)
- PP-34 Crystal structure, Hirshfeld surface analysis and three-dimensional frameworks and molecular docking studies: Derivatives of Norephedrine; Part (I)
E. Şahin, E. N. Ozkan, Ö. Gundogdu Aytaç (Erzurum/TR)
- PP-35 Novel zwitterionic molecular structure of a barbiturate salt and DFT study (nnp-143)
A. Mahmoodi, E. Nemati-Kande (Urmia/IR), T. Tunç (Aksaray/TR), E. Şahin (Erzurum/TR), N. N. Pesyan (Orumiyeh/IR)
- PP-36 Two novel Cu/Ce complexes: crystal structures and their properties
A. Koščiková (Košice/SK), M. Tomás, I. Ara, L. R. Falvello (Zaragoza/ES), J. Černák (Košice/SK)
- PP-89 “Hexagonal” Perovskites: From Stacking Sequence to Space Group Symmetry and New Opportunities
O. Clemens (Stuttgart/DE)

- PP-90 Synthesis and Structural Characterisation of An Elusive, Organometallic Gallium Monofluoride Complex via Single-Crystal-Based Reactivity
J. Stephan (Garching/DE)
- PP-93 U3 Unveiling the Unseen and Undetectable: Automated Electron Diffraction and its growing role in solid state characterization
G. Santiso-Quinones (Allschwill/CH)

Frontier Molecular Crystallography and Supramolecular and Framework Structures

- PP-37 Advanced crystallisation methods for SC-XRD
N. Nöthling, M. Turberg (Mülheim an der Ruhr/DE)
- PP-38 Crystallography in Synergy: Updates on Rigaku Single-Crystal Instrumentation
C. J. Schürmann, K.-N. Truong, J. Wojciechowski, E. Buchsteiner, F. White (Neu-Isenburg/DE)
- PP-39 The molecular und crystal structure of Durene: X-ray diffraction using a non-spherical approach and quantum chemical investigations of its weak intermolecular interactions
G. J. Reiss (Düsseldorf/DE), I. S. Konovalova (Düsseldorf/DE, Kharkiv/UA)
- PP-40 Maximized Efficiency in MOF/COF Structure Analysis
C. Wolf, T. Stürzer, A. Lübben, T. Dunaj (Karlsruhe/DE)
- PP-41 Pillarplex SOCs: Rim-Functionalizations as Achor Points for Further Tailored Modifications
J. Preinl (Garching/DE)

Crystal Physics

- PP-42 Empirical electronic polarizabilities of iodine (I⁻) and bromine (Br⁻, Br⁷⁺) for the prediction of refractive indices
S. Nezamabadi, R. X. Fischer (Bremen/DE)
- PP-43 High-pressure polymorphism in SnI₄
K. Fuchizaki (Matsuyama/JP), A. Suzuki (Sendai/JP), I. Rietveld (Rouen/FR)
- PP-44 Elastic and piezoelectric properties of Bi₁₂GeO₂₀ and Bi₁₂TiO₂₀ at high temperatures
D. Werner, E. Haussühl, B. Winkler (Frankfurt a. M./DE)

PP-45 Coexisting antiferromagnetic phases on the frustrated pyrochlore sublattice of the mixed Jahn-Teller system $\text{Ni}_{1-x}\text{Cu}_x\text{Cr}_2\text{O}_4$
M. Tovar, M. Reehuis, B. Klemke, D. M. Töbrens, J.-U. Hoffmann,
 A. Hoser (Berlin/DE)

PP-46 High-Temperature Stability and the ~460 K Anomaly in Fresnoite probed by Resonant Ultrasound Spectroscopy and Dilatometry
 E. Haussühl (Frankfurt a. M./DE)

Mineralogical Crystallography

PP-47 CO₂ sequestration using waste concrete in future building applications: unravelling elemental structural implications
C. Rüscher, S. J. Akinbodunse, S. Tome (Hanover/DE)

PP-48 Crystal-chemical factors influencing Eu(II) luminescence in solid-state metal hydrides
H. Kohlmann, A. Nain, L. Millahn, M. Gebauer, L. Schmidt (Leipzig/DE)

Functional Materials 1

PP-58 Enhanced removal of hexavalent chromium using pine needle-derived activated carbon modified with NiO and $\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$: Characterization and adsorption behavior
 S. Kouvalakidou, A. A. Thysiadou (Kavala/GR), I. Konstantinou (Ioannina/GR),
 A. K. Tolkou, G. Z. Kyzas (Kavala/GR)

PP-59 Synthesis and characterization of hybrid modified activated carbons from olive stones for the removal of Cr(VI) from water
A. K. Tolkou, A. A. Thysiadou, K. N. Maroulas (Kavala/GR),
 I. Konstantinou (Ioannina/GR), G. Z. Kyzas (Kavala/GR)

Aperiodic and Complex Structures and Structure Property Relationships

- PP-49 Competing Charge Density Waves in Pressurized SmNiC_2
A. Eich, A.-A. Haghighirad, A. von Ungern-Sternberg Schwark,
M. von Westarp (Karlsruhe/DE), G. Garbarino (Grenoble/FR), M. Le Tacon,
M. Merz, S.-M. Souliou (Karlsruhe/DE)
- PP-50 $\text{Na}_{25}(\text{Cd}_x\text{Hg}_{1-x})_{52}$ ($x=0.252$): A new complex sodium metallide at the
pseudo-binary section ' NaCd_2 '-- NaHg_2
I. Junker, C. Röhr (Freiburg i. Br./DE)
- PP-51 Phase diagram of and quantum criticality in $\text{Sc}(\text{V}_{1-x}\text{Cr}_x)_6\text{Sn}_6$
M. Merz, N. Maraytta (Karlsruhe/DE), X. Mi, X. Chen (Chongqing/CN),
F. Hardy, L. Wang, C. Meingast (Karlsruhe/DE), A. Wang, Y. Chai,
M. He (Chongqing/CN)
- PP-52 Combining single crystal diffuse scattering and *ab initio* molecular dynamics
simulations to understand framework dynamics in $\text{AlPO}_4\text{-5}$
E. M. Schmidt, M. Fischer (Bremen/DE)
- PP-54 Single-crystal growth and characterisation of the kagome material CeFe_6Ge_6
M. Schulze, E. Carrillo-Aravena, T. Doert, M. Ruck (Dresden/DE)
- PP-55 Structural and spectroscopic characterizations of mullite-type $\text{PbAl}_{1-x}\text{Fe}_x\text{BO}_4$
M. M. Murshed, T. M. Gesing (Bremen/DE)
- PP-56 Crystallography and mechanical properties of $\tau_2\text{-Al}_3\text{FeSi}$
L. Richter, A. Leineweber (Freiberg/DE)
- PP-57 Cation mutation in chalcogenide semiconductors as a path towards
CRM-free top absorber layer for tandem solar cells
G. Gurieva, D. M. Többens (Berlin/DE), M. Pilvet (Tallinn/EE),
A. Manjon Sanz (Oak Ridge, TN/US), M. Avdeev (Lucas Heights/AU),
M. Kauk-Kuusik (Tallinn/EE), S. Schorr (Berlin/DE)

Functional Materials 2

- PP-60 Influence of electrolyte solvents on the intercalation reaction of Na^+ into ZrS_2 and HfS_2 host structures
L. Liers, S. Mangelsen, M. Behrens (Kiel/DE)
- PP-61 Synthesis and characterization of spinel-type compounds AM_2O_4 (A: Zn^{2+} , Cu^{2+} , M: Fe^{3+} , Ga^{3+}) with different average crystallite sizes (ACS) as tailored visible-light photocatalysts
M. Lovino Nocetti (Bremen/DE), A. Wollbrink (Essen, Bremen/DE), T. M. Gesing (Bremen/DE)
- PP-62 Phase segregation of end-of-life nickel-rich layered lithium transition metal oxide cathodes: implications for direct regeneration
C. Zamparas, E. Eiche, J. Kolb (Karlsruhe/DE)
- PP-63 Synthesis and Optical Characterization of (Nd,Pr): LiYF_4 Crystals
N. Tuvjargal, U. Nergui, D. Unurbileg, N. Tsogbadrakh (Ulaanbaatar/MN), B. Chunfeng (Hohhot/CN), J. Davaasambuu (Ulaanbaatar/MN)
- PP-64 Lithium Makes the Difference – Phase Transitions of the Lithium-Ion Conductor Li_4SnS_4
L. G. Balzat (Stuttgart, Munich/DE), S. Bette (Stuttgart/DE), J. Blahusch (Stuttgart, Munich/DE), C. Schneider, I. Moudrakovski, K. Gjorgjevikj (Stuttgart/DE), S. Krause (Stuttgart, Ulm/DE), B. V. Lotsch (Stuttgart, Munich/DE)

Synthesis-structure / non crystalline/disordered materials

- PP-65 Microstructural, Electrochemical and Mechanical Behavior of Cold-Worked and Heat-Treated AISI 316Ti Stainless Steel in Aggressive Acidic Media
H. Kaddour (Alger, Bab ezzouar/DZ)
- PP-66 Understanding the nature of Cu- and Mg-oxides in Cu/MgO catalyst systems
B. Taetz, S. Mangelsen, M. Behrens (Kiel/DE)
- PP-67 Mesoscale architecture of gadolinium and cobalt doped cerium oxide hierarchical catalyst
P. Woźniak (Wrocław/PL)
- PP-68 Structural Studies of Substituted Polycrystalline $\text{Na}_3\text{Co}_{2-x}\text{Ni}_x\text{SbO}_6$ Antimonates
M. Gorbunov, B. Schwarz, D. Mikhailova (Eggenstein-Leopoldshafen/DE)

- PP-69 Modelling stacking disorder in $\text{Fe}(\text{C}_2\text{O}_4) \cdot 2\text{H}_2\text{O}$
S. Mangelsen, M. Chumakovski, M. Behrens (Kiel/DE)
- PP-70 Structure of a deep eutectic solvent, a mixture of proline and glycerol, from X-ray and neutron diffraction
C. Garvey, B. Becks (Garching/DE), G. Bryant, S. Bryant (Melbourne/AU), S. Rouziere (Orsay/FR), T. Hughs, Y. Zhang (Chilton/GB)
- PP-71 Sintered diamond and wBN alloy using a combination of shock and static high pressure
M. Araki (Handa/JP)
- PP-91 Advancing PDF Analysis: Fast and High-Quality Local Structure Insights with XRDynamic 500
M. Kremer, T. Faske, P. Vir, B. Schrode (Graz/AT)

Young Crystallographers: Lightning talks

- PP-72 PDF analysis of amorphous calcium and magnesium carbonates at high pressures
L. Wedek, L. Bayarjargal (Frankfurt a. M./DE), C. Prescher, C. Otzen, (Freiburg i. Br./DE), K. Glazyrin (Hamburg/DE), B. Winkler (Frankfurt a. M./DE)
- PP-73 $\text{Cs}_{14}\text{Hg}_{17}\text{O}_4$ – a new cesium mercuride oxide with a previously unknown $[\text{Hg}_{18}]$ cluster
T. Xu, C. Hoch (Munich/DE)
- PP-74 Crystal structures of $\text{Cs}_{18.5}\text{Rb}_{0.5}[\text{AlO}_4]_2[\text{Hg}_4]_2$ and $\text{Cs}_{26}[\text{Fe}_2\text{O}_7]_2[\text{Hg}]_8[\text{Hg}]_6$
H. Waldmann, N. Kötter, L. Nusser, C. Hoch (Munich/DE)
- PP-75 Three Polymorphic Modifications of $\text{Yb}(\text{OAc})_3$ Co-existing in the Temperature Range 200-523K: A Relation Between Orthorhombic and Hexagonal Structures
M. Zhernakov, J. Möbs, K. Müller-Buschbaum (Gießen/DE)
- PP-76 Crystallographic Insights into the Stereoselectivity of Methionine Adenosyltransferases
M. Bolz (Brunswick/DE), L. Gericke, J. Andexer (Freiburg i. Br./DE), W. Blankenfeldt (Brunswick/DE)
- PP-77 Structural Insights into the ADP Ribosyltransferase (ARR) from *Mycobacterium smegmatis* and the Implications for Inhibitor Search
L. von Soosten (Hamburg/DE)

- PP-78 $\text{Ba}_{21}\text{N}_5(\text{MnN}_3)_2$ – a new ternary subnitridometalate
L.-V. Pietsch, C. Hoch (Munich/DE)
- PP-79 Crystallographic fragment screening towards new NS2B-NS3 Zika protease inhibitors
L. S. Benz, J. Wollenhaupt, M. Oelker (Berlin/DE), A. Jirgensons (Riga/LV), T. Miletic, U. Müller, M. S. Weiss (Berlin/DE)
- PP-80 Low-Cost Crystallization Automation for Cationic Metallocavitands (Pillarplexes)
M. Saviak, J. Zuber, L. Richter, A. Pöthig (Garching/DE)
- PP-81 Cryo and room temperature (RT) serial synchrotron crystallography (SSX) reveals binding modes of previously unexplored β -lactam antibiotics
G. Gore, A. Prester, D. von Stetten, K. Bartels, E. C. Schulz (Hamburg/DE)
- PP-82 High-throughput structural investigation of Cu content-dependent second phase formation in $(\text{Mn,Fe,Co,Ni,Cu})_3\text{O}_4$ thin film materials libraries
V. Strotkötter, A. Kirsch, A. Ludwig (Bochum/DE)
- PP-83 Exploring compositional space in non-equi-molar high entropy spinel oxides
C. F. Eugenio (Bochum/DE, Bogotá/CO), S. C. Sánchez (Bogotá/CO), A. Kirsch (Bochum/DE)
- PP-84 Reference Database for Chemical Bonding Analysis
F. Bartley, F. Kleemiß (Aachen/DE)
- PP-85 Capturing Spin Transitions in Crossover Complexes *via* Quantum Crystallographic Disorder Refinement
D. Brück, F. Kleemiß (Aachen/DE)
- PP-86 Porous Pillarplex Materials: Towards Gas Adsorption in the Solid State
J. Zuber, A. Heidecker, A. Pöthig (Garching/DE)
- PP-87 Crystal architecture through energetic insights: 2,6-bis(4*H*-1,2,4-triazol-4-yl) pyridine hydrate
M. G. Bogdanović (Novi Sad/RS), I. S. Konovalova (Düsseldorf/DE, Kharkiv/UA), G. J. Reiss (Düsseldorf/DE), M. V. Rodić (Novi Sad/RS)



SOCIAL PROGRAMME

Welcome reception

Join us for an opportunity to reconnect with old colleagues and meet new faces in a relaxed atmosphere. Let's unwind together over snacks and drinks, share our first impressions, and get in the perfect mood for the exciting days ahead!

Date	Wednesday, 25 February
Time	19:15–21:15
Fee	included in the conference fee, accompanying person EUR 25
Location	Foyer, industrial exhibition

Social evening

The last evening of the conference will be celebrated at the elegant Radisson Blu Senator Hotel in Lübeck. Participants can look forward to a pleasant evening in a festive setting, offering opportunities for exchange, networking, and relaxed conversation. Enjoy the exquisite atmosphere of the hotel and end the day in good conversation. An unforgettable conclusion to an inspiring conference.

Date	Friday, 27 February
Time	19:00–23:00
Fee	EUR 75 (Congress participants/Students/ Accompanying persons)
Location	Radisson Blu Senator Hotel Willy-Brandt-Allee 6 23554 Lübeck

All participants may arrange transport themselves.



28th Congress and General Assembly of the International Union of Crystallography

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YOUNG CRYSTALLOGRAPHERS

Young Crystallographers at DGK 2026 – Join Us!

The Young Crystallographers (DGKYC) warmly invite you to three engaging sessions dedicated to early-career researchers in the dynamic and interdisciplinary field of crystallography. Whether you are presenting, networking or simply curious to learn more, these sessions offer an exciting platform to exchange ideas and connect with peers.

Microsymposium 1: Lightning talks

We kick off with 16 fast-paced lightning talks, where young crystallographers will present their research in concise, 5-minute snapshots. These presentations serve as an introduction to their work and provide a springboard for deeper discussions at their respective posters. Get ready for a rapid-fire tour of the latest developments all around crystallography!

Date: Wednesday, 25 February

Time: 15:45–17:05

Room: AM 1

Get Together of the Young Crystallographers (for young Crystallographers only!)

What would a DGK meeting be without a dedicated Young Crystallographers networking event? Join us for an interactive session where we will update you on DGKYC activities, elect a new Co-Chair, and share exciting news about upcoming initiatives. After the formalities, enjoy the opportunity to meet fellow young crystallographers over drinks and snacks in a relaxed setting.

Date: Thursday, 26 February

Time: 19:45–21:00

Room: AM 2

Lieselotte-Templeton Awards Session

We are honored to host a special session featuring the recipients of the prestigious Lieselotte-Templeton Prize 2026. Each awardee will share key insights from their prize-winning thesis, offering a deeper dive into groundbreaking contributions to the field. This session is a must-attend for those looking for inspiration from some of the brightest young minds in crystallography.

We look forward to welcoming you to one, two, or all three of these sessions—see you there!

For the Young Crystallographers,
Florian Meurer, Anushka Ghosh and Ben Ebel

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MEETING OF THE WORKING GROUPS

Thursday, 26 February | 19:45-21:00

AK 1 Young Crystallographers – JKYC
AM 2 The meeting of AK 1 will take place during the Get Together of the Young Crystallographers.

Friday, 27 February | 12:15-13:00

AK 6 Chemical Crystallography
AM 1

AK 3 Experimental Methods
AM 2

AK 4 Theoretical Methods
AM 3

AK 2 Teaching of Crystallography
AM 4

Friday, 27 February | 17:15-18:00

AK 5 Biological Crystallography
AM 1

AK 9 Materials Science Crystallography
AM 2

AK 7 Physical Crystallography
AM 3

AK 8 Mineralogical Crystallography
AM 4

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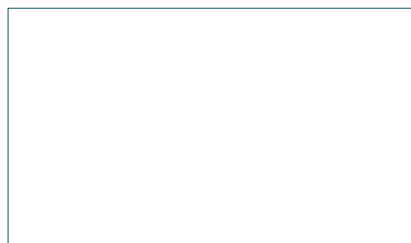
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GENERAL INFORMATION

**Conference language**

The conference language is English.

**Opening hours**

	Wednesday	Thursday	Friday	Saturday
Check-In	12:30–19:30	08.45–18:15	08:15–18:00	08:30–12:00
Industrial exhibition	12:30–21:30	10:00–18:00	09:00–17:30	08:30–12:30

**Publication of abstracts**

All abstracts will be published in the abstract book and will be available on the conference homepage.

**Certificates of attendance**

Certificates of attendance will be sent automatically after the conference to the e-mail address used for registration.

**Internet**

The University of Lübeck has free Wi-Fi that can be used throughout the building. Upon request and after registering on a list (name and signature), each participant will receive an individual access code at check-in.

**Catering**

During the breaks, there will be a small selection of fruit and snacks as well as coffee and tea. Lunch will be provided on a self-pay basis by the Mensa Lübeck opposite the Audimax at Mönkhofer Weg 241. Please note that only card payment (EC, Visa and MasterCard) is possible. It is not possible to pay in cash at the counters. Water dispensers will be available at the conference venue. For the sake of the environment: Please bring refillable water bottles.

You can also take advantage of the following catering options:

- Bakery „Junge Die Bäckerei.“
Monday to Friday from 07:00 to 18:30, Saturday from 07:00 to 18:00
- Café Curie
Monday to Friday from 08:00 to 18:00
- Campus Suite/Campus Taste
Monday to Friday from 08:00 to 18:00
- Café Lounge „Bits + Bytes“
Monday to Thursday from 07:45 to 14:30, Friday from 07:45 to 14:00

You can find detailed directions and the web addresses of the different shops on the conference website. Simply scan the QR code for easy access.





Cloakroom

There is a cloakroom in the basement (UG). You can reach these via the stairs.

Attention: the lift in the building is currently out of order and cannot be used.

Please note that the cloakroom is unattended and therefore we cannot accept any responsibility or liability for clothing and items left there.



General Assembly 2026

The DGK General assembly will take place on Thursday, 26 February in AM 1 at 17:45–19:45. We kindly invite all members to attend!

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CRYSTALLOGRAPHIC MEETING
2027

INDUSTRIAL SYMPOSIUM

Thursday, 26 February

12:15–13:15 Bruker AXS SE (Karlsruhe/DE)

AM 1

New Developments in Structural Research

Tobias Dunaj, Michael Evans, Florian Stemme,
Anna Lübben (Karlsruhe/DE)

Join us for an engaging session where you can network with other users and our experts, share insights, and stay ahead of the curve in structural research. We look forward to welcoming you.





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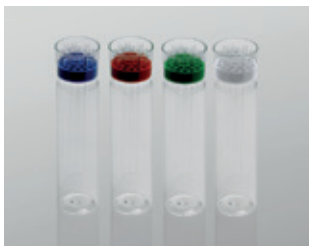


XRD flow capillary with Luer-lock

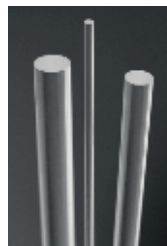


NEW

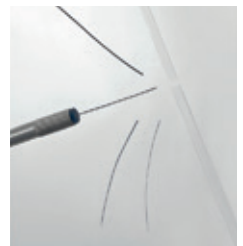
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FIZ Karlsruhe (Eggenstein-Leopoldshafen/DE)	5
Hilgenberg GmbH (Malsfeld/DE)	15
Huber Diffraktionstechnik & AXO Dresden (Rimsting/DE)	2
International Union of Crystallography	14
IUCr 2029	13
Malvern Panalytical GmbH (Kassel/DE)	7
Oxford Cryosystems Ltd (Long Hanborough/UK)	8
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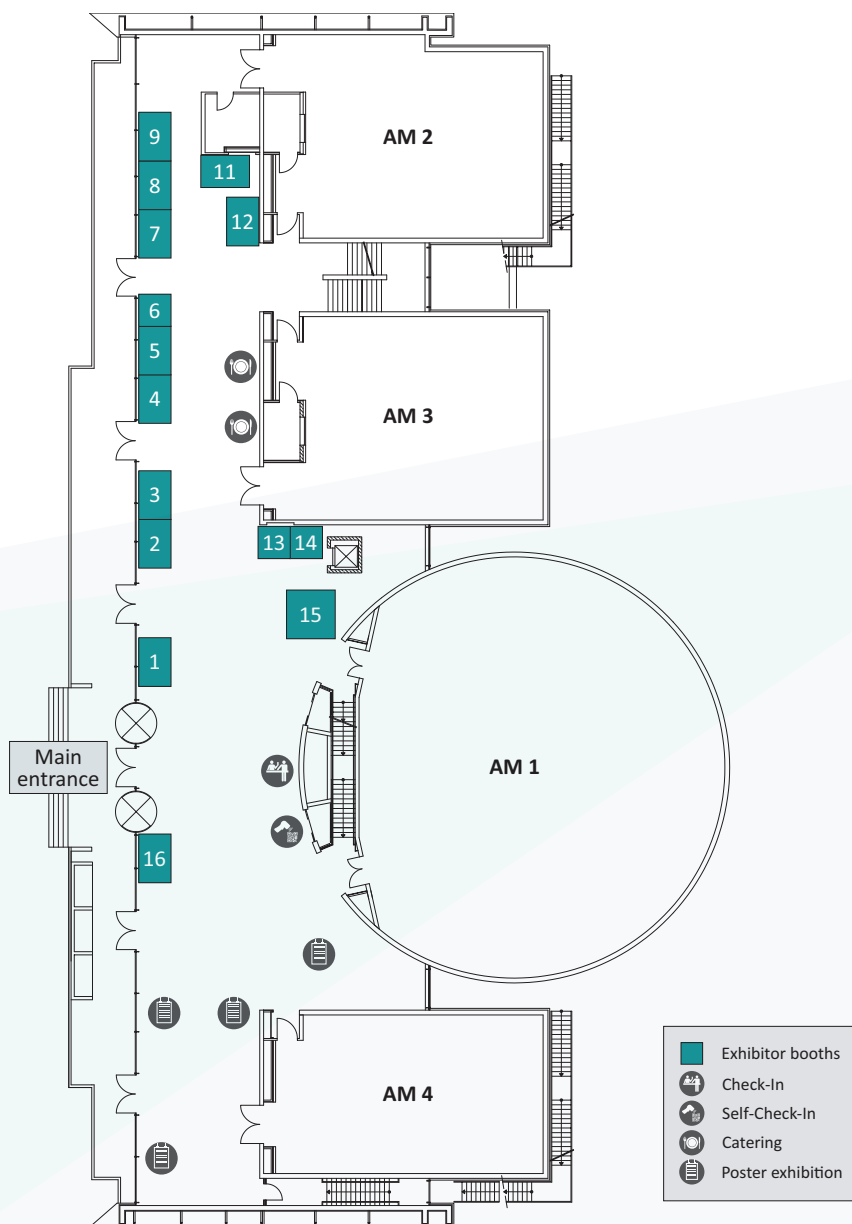
Media collaborations

Condensed Matter
MDPI

Elements – An international magazine of mineralogy, petrology, and geochemistry
Elements

Journal of Chemical Crystallography
Springer Nature

State at printing.



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INDEX OF PLENARY SPEAKERS, AUTHORS AND CHAIRS

A

Adam, M.	19, 22
Adams, F.	16
Ade, M.	36
Adouar, I.	21
Agthe, M.	13
Akbar, F. I.	17, 35
Akhundov, I.	30
Akilli, R.	35
Akinbodunse, S. J.	38
Andexer, J.	12, 41
Angst, M.	27
Ara, I.	36
Araki, M.	41
Arhangelskis, M.	20
Aroyo, M. I.	30
Aslandukov, A.	36
Atata, S. B.	15
Austin, R.	23
Avdeev, M.	39

B

Bachmann, H.	34
Balzat, L. G.	40
Bartel, S.	35
Bartels, K.	12, 42
Barthel, T.	34
Barthelmess, M.	19
Bartley, F.	13, 42
Bastick, K. A. C.	19
Bayarjargal, L.	11, 15, 22, 35, 41
Bazzi, S.	23
Beck, T.	16, 18, 19, 27
Becks, B.	41
Beddard, G.	27
Behrens, M.	40, 41
Benz, L. S.	12, 34, 42
Berking, T.	36
Bette, S.	16, 20, 21, 28, 40
Bickermann, M.	15
Bílá, Š.	14
Bílý, T.	14
Binder, S.	23
Blahusch, J.	40
Blakeley, M. P.	14
Blankenfeldt, W.	12, 41
Bloch, Y.	13

Blukis, R.	15
Bock, B.	36
Bock-Bierbaum, T.	27
Bockfeld, D.	36
Bode, H.	23
Bodensteiner, M.	14, 20, 28, 31
Bogdanović, M. G.	13, 42
Boger, J.	14
Bojarska, J.	13
Bolz, M.	12, 41
Bömer, C.	14
Bon, V.	20
Borisov, A.	25
Bosman, R.	26
Botha, S.	26
Bourenkov, G.	13, 27
Bourhis, L.	16
Boyakova, Y.	27
Breithaupt, C.	20
Breternitz, J.	17, 30
Brinkmann, M. M.	34
Brummerstedt Iversen, B.	18
Brüning, L.	35
Brützam, M.	15
Brüx, D.	13, 42
Bryant, G.	41
Bryant, S.	41
Buchsteiner, E.	22, 37
Bücker, R.	22
Bull, C.	20
Bungarten, J.	35
Bykov, M.	17, 35
Bykova, E.	24, 25, 35

C

Calamiotou, M.	15
Carrillo-Aravena, E.	39
Carvajal, E.	33
Celani, P.	33
Cerantola, V.	25
Černák, J.	36
Chai, Y.	39
Chapman, H.	19
Chariton, S.	33
Charkin, D.	25
Chatzieftymiou, S. D.	13, 19
Chen, X.	39

INDEX OF PLENARY SPEAKERS, AUTHORS AND CHAIRS

Chernyshov, D.	27	Elsner, N. G.	17
Chintakindi, H.	26	Enax, J.	25
Chodkiewicz, M.	13, 20	Engel, K.	36
Chretien, A.	26	Epple, M.	24, 25
Christian, P.	34	Estengre Pérez, J.	27, 34
Chumakovski, M.	41	Estévez Rams, E.	33
Chunfeng, B.	40	Etter, M.	20, 22
Chuvashova, I.	33	Eugenio, C. F.	12, 42
Clemens, O.	37	Evans, M.	52
Cocomazzi, G.	25		
Colsmann, A.	24	F	
Corkett, A.	17	Falke, S.	19
		Falvello, L. R.	36
D		Fang, H.	19
Da Cruz, Q.	35	Fatima, H.	34
Da Silva, P.	27	Fernandes Ligorio, R.	14
Damjanovic, T.	33	Fernandez-Cuesta, I.	34
Danziger, M.	26	Figueiredo, J.	28
Das, H.	16	Fischer, M.	24, 39
Datta, R.	24	Fischer, P.	19
Daub, M.	36	Fischer, R. X.	37
Davaasambu, J.	40	Folkers-Karlsson, L. C.	33
de Diego Martinez, I.	14	Franta, Z.	14
de la Flor, G.	30	Fraunhofer, C.	17
de Wijn, R.	26	Frey, W.	36
Deger, S.	36	Friese, K.	15, 17, 27
Dey, S.	26	Fritz, G.	34
Dincă, G.	35	Fuchizaki, K.	21, 37
Dinnebier, R. E.	16, 21	Fuhrmann, P.	30
Doert, T.	24, 33, 39		
Dominiak, P.	13	G	
Dunaj, T.	19, 29, 33, 37, 52	Gajda, R.	20
		Gajdos, L.	14
E		Galchenkova, M.	19
Ebbinghaus, S. G.	16	Gaman, C. D.	27
Ebel, B.	11, 24	Ganguly, R.	23, 35
Effenberger, H.	35	Ganschow, S.	15
Effert, J.	23	Garbarino, G.	39
Ehrling, S.	20	García Medina, K.	15, 33
Ehrt, C.	19	Gardelis, S.	15
Eich, A.	39	Garvey, C.	41
Eiche, E.	40	Gasharova, B.	27
Eigner, V.	26	Gebauer, M.	38
El Bali, B.	21	Geibel, S.	23
Elagouri, N.	35	Gellner, J.	23
Elcoro, L.	30	Genter-Dieguez, C.	27
Elinjikkal, D.	19	Gericke, L.	12, 41

INDEX OF PLENARY SPEAKERS, AUTHORS AND CHAIRS

Gerteis, F.	19	Hoch, C.	11, 12, 24, 41, 42
Gesing, T. M.	39, 40	Hoell, A.	20
Geßner, J.	16	Hoffmann, A.	15
Geyer, M.	23	Hoffmann, J.-U.	38
Gimferrer, M.	14	Holstein, J. J.	19, 27
Giordano, N.	24	Holyńska, M.	35
Gjorgjevikj, K.	40	Hölzel, M.	20
Glazyrin, K.	11, 25, 41	Holzheid, A.	25
Göb, C.	22	Hoser, A.	38
Gorbunov, M.	40	Hübner, J.-M.	31
Gore, G.	12, 42	Huc, I.	23
Graeser, S.	35	Hughs, T.	41
Grandgirard, C.	13	Hüppe, H.	27
Grebentsov, A.	13	Huseyn-zada, N.	20
Groll, M.	23		
Grüne, T.	16, 18, 22	I	
Gruzinov, A.	13	Inckemann, S.	15
Grzechnik, A.	15, 17, 27	Inoue, S.	36
Gugushev, C.	15	Irmer, E.	18, 29
Gumprecht, L.	19		
Gundoğdu Aytaç, Ö.	36	J	
Günther, S.	19	Jacobs, J.	16
Guo, J.	28	Jafari, S.	13
Gurieva, G.	25, 26, 39	Jandl, C.	24
		Jarošová, M.	26
H		Jasnowski, M.	22
Hagelueken, G.	23	Jensen, K. M. Ø.	17
Hagemann, A.	34	Jirgensons, A.	12, 42
Häger, M.	17	Junker, I.	39
Haghighirad, A.-A.	39		
Hajdu, J.	14	K	
Hakanpää, J.	13, 18, 19	Kaddour, H.	40
Hamdi, F.	14	Kahlenberg, V.	16
Hardy, F.	39	Kaila, V.	23
Hartenfels, J.	36	Karničar, K.	19
Hauf, C.	20	Kaskel, S.	20
Haussühl, E.	15, 37, 38	Kastritis, P. L.	14
He, M.	34, 39	Kauk-Kuusik, M.	39
Heidecker, A.	13, 42	Kehr, J.	33
Heidler, T.	23	Kehrenberg, M. C.	34
Hekstra, D.	27	Khakurel, K.	14
Hempelmann, G.	24	Kierspel, T.	33
Hennig, C.	20	Kirsch, A.	12, 17, 25, 29, 42
Herbst-Irmer, R.	14, 16, 18, 29	Klaubert, T.	23
Herradi, S.	21	Kleeberg, C.	36
Herzog, A.-M.	34	Kleemiß, F.	13, 14, 18, 30, 42
Hirscher, M.	16	Klemke, B.	38

INDEX OF PLENARY SPEAKERS, AUTHORS AND CHAIRS

Kloß, S. D.	17	Lieske, J.	19
Klureza, M.	27	Locke, R. J. C.	36
Knapp, S.	19, 27	Longa, C.	25
Kochel, A.	35	Loos, M.	23
Kohlmann, H.	17, 38	Lorenzen, K.	26
Kolb, J.	40	Loriga Jr., R.	33
Kollewe, M.	27	Lotsch, B. V.	28, 40
Konovalova, I. S.	13, 30, 37, 42	Lovino Nocetti, M.	40
Konstantinou, I.	38	Loza, K.	24
Koohgard, M.	36	Lübben, A.	19, 22, 29, 33, 37, 52
Korn, S.	20	Ludwig, A.	12, 42
Kortman, H. M.	19	Luebben, J.	29, 33
Koščíková, A.	36	Luiz Alves Jardim, F.	28
Kostka-Wirtz, K.	24	Lyu, J.	35
Kötter, N.	11, 41		
Kottke, T.	26	M	
Kouvelakidou, S.	38	Macchi, P.	22
Kovalev, K.	13	Madariaga, G.	30
Kovalev, V.	24, 25	Madsen, A.	33
Krause, S.	40	Mahmoodi, A.	36
Krawczuk, A.	14, 22, 30	Mahmoudi, S.	22
Krebs, D.	14	Makovicky, E.	35
Kremer, M.	41	Mancuso, A.	26
Kuchta, B.	20	Mandal, P.	23
Kulik, M.	13	Mangelsen, S.	40, 41
Kümmel, D.	35	Manjon Sanz, A.	39
Kung, J. C. K.	33	Mann, D.	23
Kyzas, G. Z.	38	Manousou, D.	15
		Maraytta, N.	39
L		Maroulas, K. N.	38
Łach, G.	20	Martin, J. D.	20
Lachkar, M.	21	Mathis, Y.-L.	27
Langer, N.	17	Mazur, B.	20
Le Tacon, M.	39	Meents, A.	19
Lehmann, C. W.	14, 33	Mehrabi, P.	26
Leimkohl, J.-P.	27	Meingast, C.	39
Leineweber, A.	30, 39	Melgalvis, D. M.	33
Leisegang, T.	17, 26	Merkelbach, J.	24
Lenczyk, C.	29	Merkulova, O.	13
Lennartz, F.	27, 34	Merz, M.	39
Li, X.	25	Meurer, F.	11, 20, 31
Li, Y.	23	Meven, M.	20, 22
Lí, Y.-M.	26	Meyer, D. C.	31
Liang, J.	22	Meyer, J.	19
Liddle, S. T.	31	Meyer, M.	22
Liermann, H.-P.	25	Mi, X.	39
Liers, L.	40	Mikhailova, D.	26, 40

INDEX OF PLENARY SPEAKERS, AUTHORS AND CHAIRS

Rejnhard, P.	20	Schulze, T.	19
Rekis, T.	33	Schulze zur Wiesche, E.	25
Reuter, T. H.	15, 22	Schürmann, C. J.	22, 37
Richert, C.	36	Schwarz, B.	40
Richter, L.	12, 39, 42	Schweinle, C.	36
Richter, L.	12, 39, 42	Schwung, S.	15
Ridley, C.	20	Sedykh, A.	26
Rietveld, I.	37	Seeberger, P. H.	19
Rittmann, D. C.	34	Seifert, L. M.	30
Rodić, M. V.	13, 42	Senst, J.	19
Rodrigues, A. C.	19	Senyshyn, A.	20
Röhm, H.	24	Shahed, H.	27
Röhr, C.	35, 36, 39	Shahzad, S.	23
Römer, E.-E.	27	Shaikhqasem, A.	14
Rouziere, S.	41	Sharapova, N.	24, 25, 35
Ruck, M.	39	Shevchenko, A.	21
Ruiz Carrillo, D.	13	Sicher, P.	17
Runge-Seither, G. L.	36	Simon, P.	22
Rüscher, C.	38	Singh, P.	27
Rybicka, P.	13	Sławiński, W.	20, 21
Rytz, D.	15	Sleptsova, A.	16
		Smith, V.	19
		Smitha, S.	33
S		Sohn, Y. J.	15
Şahin, E.	36	Sornaly, F. A.	34
Sánchez, S. C.	12, 42	Souliou, S.-M.	39
Santiso-Quinones, G.	24, 37	Soumitra, P.	35
Sarkar, P.	16	Spahr, D.	24, 25, 35
Saviak, M.	12, 42	Span, I.	23, 35
Sayyad, S.	23	Stam, D.	24
Schenkman, L.	34	Stegmann, D.	34
Schikora, H.	27	Steinfeld, G.	24
Schleid, T.	36	Stemme, F.	52
Schmidt, E. M.	24, 39	Stephan, J.	37
Schmidt, L.	38	Steuber, J.	34
Schneberger, N.	23	Stöger, B.	30
Schneider, C.	40	Strapasson, G. B.	17
Schneider, T. R.	13	Strotkötter, V.	12, 42
Schorr, S.	16, 20, 24, 25, 26, 39	Stubbs, M. T.	14, 20
Schreuer, J.	15	Stürzer, T.	22, 29, 37
Schröck, C.	22	Suzuki, A.	37
Schröder, C.	22	Szal, T.	19
Schubert, R.	26		
Schulz, E. C.	12, 25, 26, 42	T	
Schulz, J.	26	Taetz, B.	40
Schulz, N.	19	Tamm, M.	36
Schulz, T. F.	34	Tasci, E.	30
Schulze, M.	39		

INDEX OF PLENARY SPEAKERS, AUTHORS AND CHAIRS

Tchoń, D.	22	W	
Tellkamp, F.	27	Wagner, P.	20
Terban, M. W.	21	Waldmann, H.	11, 41
Teuber, J.	34	Wang, A.	39
Thekku Veedu, S.	19	Wang, L.	39
Thiele, G.	24	Wang, Y.	35
Thorn, A.	16, 18	Weber, G.	23, 27
Thysiadou, A. A.	38	Wedek, L.	11, 41
Tittmann, K.	35	Weidenthaler, C.	16
Többens, D. M.	16, 24, 38, 39	Weil, M.	18
Toimil-Molares, M. E.	22	Weiss, M. S.	12, 27, 33, 34, 42
Tolkou, A. K.	38	Weißenburg, A.	34
Tomás, M.	36	Wendorff, M.	35
Tome, S.	38	Werner, D.	37
Topa, D.	35	White, C.	11
Tovar, M.	38	White, F.	22, 37
Trautmann, C.	22	Wilmes, S.	35
Triandafillidis, D. P.	33	Windshügel, B.	19
Truong, K.-N.	22, 37	Winkler, B.	11, 15, 22, 24, 25, 35, 37, 41
Tsipas, P.	15	Wojciechowski, J.	22, 37
Tsogbadrakh, N.	40	Wolf, C.	37
Tuma, R.	14	Wolf, W.	13
Tunç, T.	36	Wolfflehner, T.	18
Turberg, M.	37	Wollbrink, A.	40
Turk, D.	19	Wollenhaupt, J.	12, 42
Tuvjargal, N.	40	Wozniak, K.	20
Tzifas, I.	22	Woźniak, P.	40
U		X	
Uetrecht, C.	33	Xu, F.	23
Unurbileg, D.	40	Xu, T.	11, 41
V		Y	
Vallinayagam, M.	31	Yorke, B.	27
Vering, J.	34		
Virovets, A.	14	Z	
Voigt, J.	27	Zamparas, C.	40
Völkel, C.	19	Zanchet, D.	17
von Bahder, S.	26	Zeno, M.	34
von Soosten, L.	12, 41	Zhang, Y.	41
von Stetten, D.	12, 13, 26, 27, 42	Zhernakov, M.	11, 41
von Ungern-Sternberg Schwark, A.	39	Zhou, W.	27
von Westarp, M.	39	Zlotnikov, I.	24
Voss, K.-O.	22	Zschornak, M.	31
		Zuber, J.	12, 13, 42



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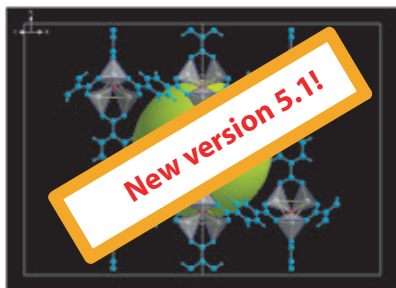
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